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Towards CFD modeling of carbon dioxide turbulent pipe line transportation

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Abstract

Safe and financially efficient pipeline transportation of carbon dioxide is a critical issue in the developing field of Carbon Capture and Storage (CCS) Technology. Presence of large and small scale structures and high Reynolds numbers in the pipeline, draw special attention to numerical simulation of turbulent material transport through the individual components of the carbon dioxide (CO₂) chain process. In this study Large Eddy Simulation (LES) of incompressible turbulent channel flow and pipe flow has been performed using OpenFoam an open source CFD tool. The results are compared with those from Direct Numerical Simulation (DNS) and the existing experimental data.

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1. Introduction

It has always been of great significance and interest to prevent CO₂ from releasing into the atmosphere. Through CCS technology which is at the moment an option to achieve the mentioned goal, Carbon Dioxide resulted from the use of fossil fuels in power generation process and other industries is transported to the geological storage sites. In this process, the most efficient transportation method would

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be through pipelines and the most economic method would be transferring CO₂ as dense fluid [1]. As a result of elevation, geometrical or hydrodynamical parameter changes it is a great challenge to keep CO₂ in the same phase along the whole pipeline. Furthermore, local changes in the thermodynamical and hydrodynamical fields, can lead to phase changes and cause vibrations and pipe material obsolescence [1].

Due to the mentioned challenges, numerical simulation of pipe line material transport is an indispensable part of the design process. Providing a deeper understanding of fluid behavior in this process, the results can be used for verification, further development and specification of the currently used experimental measurement techniques. They can also help to solve certain constructive issues and reduce or even eliminate expensive experimental test series.

In the first part of this study, turbulent channel flow has been modeled using LES for shear Reynolds number of 395 to validate the used numerical code. Grid resolution study has been conducted for One-Equation-Eddy and Dynamic Smagorinsky model for three different resolutions to choose an optimized mesh for the rest of the simulations. With the aim of selecting an appropriate LES model, three different models are implemented on a channel with the grid resolution of about 4×10^5 grid points. Mean velocity profiles and root mean square (RMS) velocity values are plotted and compared with existing DNS results reported by Moser et al. [2]. In the second part, turbulent pipe flow is modeled using Dynamic Smagorinsky model. Mean velocity is plotted and compared against existing data from experiments conducted by Zimmer et al. [3] on the Cottbus Large pipe (CoLa pipe) test facility.

2. LES of turbulent channel flow between two infinite planes

Fully developed turbulent flow in a channel has been investigated extensively in the area of wall bounded turbulence with the aim of providing deeper understanding of fluid behavior specifically near the wall. Since the first investigations in 1929 by Nikuradse and in 1938 by Reichardt, starting with mean flow studies, until today, considerable attention has been given to this area. Large number of statistics are reported through numerical simulations and experiments. The geometric simplicity and wide range of existing data make channel flow an appropriate case study for generating new numerical solvers and developing the existing ones [4].

2.1. Governing equations and numerical method

One of the most extreme difficulties in solving and analyzing turbulent flows is attributed to the wide spectrum of scales in such flows ranging from large eddies that contain most of kinetic energy of the flow to the dissipative Kolmogorov scales. Larger scales are dependent on boundary conditions and the smaller ones which are known as subgrid scales are mostly independent from the geometry and contain small portions of flow energy.

In DNS all the scales are resolved by solving Navier Stokes (N.S.) equations and none of the mentioned scales are modeled. Having access to supercomputers, it is possible now to perform DNS for simple flows and relatively high Reynolds numbers. Nevertheless, direct numerical simulation of more complicated flows and geometries at higher Reynolds numbers, as in the case of CO₂ pipe line transportation, has proven to be far more demanding than the capabilities of present supercomputers [4].

Thus, Large Eddy Simulation is chosen for this research, in which all the large scales containing most of the kinetic energy are resolved and only subgrid scales (SGS) are modeled. To decompose the mentioned scales a spatial filtering operator is applied to N.S. equations. Applying LES filter, the resolved part of a space time variable $\bar{\phi}(x, t)$ is defined by the following relation [6]:

$$\bar{\phi}(x, t) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \phi(r, t') G(x - r, t - t') dt' dr \quad (1)$$

The convolution kernel G is characteristic of the used filter. As known from Reynolds decomposition, pressure and velocity fields are decomposed to their mean values and their deviation from the mean value.

$$u = \bar{u} + u' \quad (2)$$

$$p = \bar{p} + p' \quad (3)$$

The filtered Navier Stokes equations for incompressible flow can then be defined as,

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0 \quad (4)$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\overline{u_i u_j}) = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial}{\partial x_j} \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right), \quad \overline{(u_i u_j)} = \tau_{ij}^s + \bar{u}_i \bar{u}_j \quad (5)$$

In equation (5), τ_{ij}^s is the subgrid scale Reynolds stress which represents the large scale momentum flux caused by the action of unresolved scales. The models used to estimate the SGS Reynolds stress are called subgrid scale models and solve partial differential equations to obtain the parameters needed to determine the SGS Reynolds stress [6]. The implemented SGS models in this study are introduced in chapters 2.5 and 2.6.

The simulations have been carried out for an incompressible flow, using OpenFoam (version 2.1.1), an open source CFD tool. Pressure Implicit with Splitting of Operators (PISO) algorithm has been used to solve N.S. equations for unsteady flow. The mesh has been generated using BlockMesh utility in OpenFoam. Details of the mesh configuration are discussed in the next chapter.

2.2. Computational domain and mesh configuration

In the first part, modeling of turbulent channel flow has been considered at relatively low shear Reynolds number of $Re_\tau = 395$ which is the benchmark value for the DNS carried out in [7]. The computational domain used for modeling the flow is shown in Fig. 1. Boundary conditions are selected to match the ones implemented in the benchmark used for validation [2]. No slip boundary conditions are chosen for the top and bottom walls. Periodic boundary condition is chosen in stream wise and span wise directions at which homogenous turbulence is expected, to generate fully developed turbulence. The mesh is gradually refined towards the walls to allow for close investigation of the flow near the wall. Domain size of $(4\delta \times 2\delta \times 2\delta)$ in the direction of (x, y, z) is selected with the channel half width of $\delta = 1m$ in the wall normal direction (Fig.1) to conform with the domain geometry in the used benchmark [2].

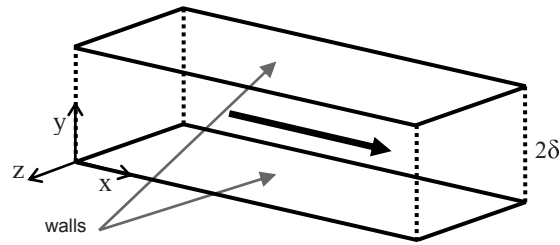


Fig.1. Channel flow geometry

2.3. Simulation setup

In order to run the simulation at the shear Reynolds number of $Re_\tau = 395$ which equals bulk Reynolds number of $Re_b = 13750$, it is essential to maintain a constant corresponding bulk velocity U_b during the runtime. The mentioned parameters are defined by the following equations where u_τ , δ , ν and τ_{wall} are friction velocity, channel half width, kinematic viscosity and shear stress at the wall respectively.

$$Re_\tau = \frac{u_\tau \delta}{\nu}, \quad Re_b = \frac{2\delta U_b}{\nu}, \quad u_\tau = \sqrt{\frac{\tau_{wall}}{\rho}} \quad (6)$$

$$U_b = \frac{1}{2} \int_{-1}^{+1} \bar{u} d\left(\frac{y}{\delta}\right) \quad (7)$$

Using the bulk velocity value and shear Reynolds number, an initial turbulent velocity field is introduced as initial condition for velocity to start the transition to turbulence. Based on the mentioned bulk velocity a pressure gradient is also calculated and it is maintained through the simulation to keep the flow running.

2.4. Averaging in time and space

To calculate the mean velocity field of the flow, to employ it later for the analysis of mean velocity profile, it is necessary to perform both time averaging and space averaging on the velocity field. The space averaging should be considered in stream wise and span wise directions at which homogeneous turbulence is expected [7]. Due to the specific temporal character of Turbulent Kinetic Energy (TKE), plotting and monitoring it will help to determine the right time for starting the averaging process. Since the average velocity in wall normal and span wise directions in channel flow are close to zero, the corresponding fluctuations can be computed and plotted easily. As it could be observed in Fig. 2, after a peak in the values of TKE at 500 seconds, their values tend to fluctuate around a fixed value. This time can be selected as a start point for averaging. Velocity field is then averaged over a time interval of about 5000 seconds to produce time averaged velocity field.

$$k = \frac{1}{2} \left(\overline{(u'_x)^2} + \overline{(u'_y)^2} + \overline{(u'_z)^2} \right) \quad (8)$$

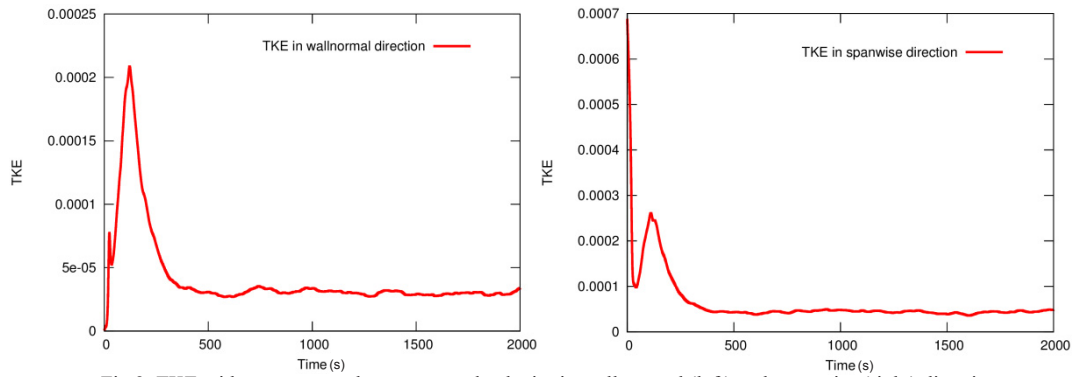


Fig.2. TKE with respect to volume averaged velocity in wall normal (left) and span wise (right) directions

2.5. Grid resolution study

With the purpose of finding an appropriate grid resolution for the channel mesh, to conserve the desired accuracy while needing a reasonable time frame for the simulation, grid resolution study has been carried out. Three different resolutions are taken into consideration ranging from a coarse one with 6×10^4 grid points to a fine one with 384×10^4 grid points. Number of cells in each direction is presented in Table (1) showing an increased refinement in each special direction. One-Equation Eddy Viscosity model is applied for this part of study which is relatively cheap in terms of needed computational time. The smallest value for nondimensional wall coordinate y^+ is presented in Table (1) for each mesh resolution.

$$U^+ = \frac{\bar{U}}{u_\tau}, y^+ = \frac{yu_\tau}{\nu} \quad (9)$$

Table 1. Grid resolution study for One-Eq. Eddy Viscosity model

Mesh type	Number of grid points	min y^+
Coarse	6×10^4 (30×50×40 in x, y, z)	1.8
Intermediate	48×10^4 (60×100×80 in x, y, z)	1
Fine	384×10^4 (120×200×160 in x, y, z)	0.48

Mean velocity profile of the turbulent flow in wall units provides appropriate insight to the fluid behavior in the vicinity of the wall and is regarded as one of the validation criteria to evaluate the efficiency and accuracy of the simulation. In Fig. 3 on the left, mean velocity profiles have been plotted in wall units for the mentioned resolutions and are compared against the existing DNS data by Moser et al. [2]. Stream wise RMS velocity which represents one of Reynolds stress components has been used as another validation factor in Fig. 3 on the right. The profiles resulted from three resolutions are compared with DNS results as well. U^+ and y^+ in these figures are nondimensional quantities which are scaled by wall variables [4]. As it can be observed, the coarse mesh is under resolved and cannot provide an acceptable agreement with DNS results. The fine mesh on the other hand was too expensive regarding the time needed for the simulation to run. Thus the mesh with 48×10^4 grid points is employed for the rest of the simulations.

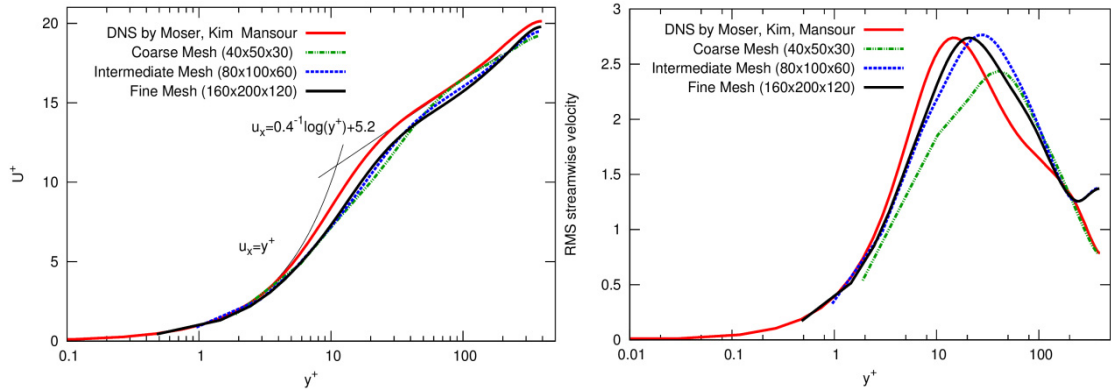


Fig.3. Grid resolution study. Mean velocity (left) and RMS stream wise velocity (right) profiles in comparison with DNS data [2] for One-Eq. eddy viscosity model

2.6. Model Study

One of the most commonly used SGS models is the one proposed by Smagorinsky in 1963. Similar to other Eddy Viscosity models, Smagorinsky model is also based on the principal that the main effects of SGS Reynolds stress are increased transport and dissipation. The SGS Reynolds stress τ_{ij}^s is expressed in terms of eddy viscosity μ_t , strain rate of the large scale \bar{S}_{ij} , filter length scale Δ and the model parameter C_s known as Smagorinsky constant. The value of C_s is not constant and can take different values in different flows. For channel flow it takes the value of about 0.065 in the bulk flow and in areas closer to the wall its value is reduced using van Driest damping function to adjust eddy viscosity in the vicinity of the wall [6]. In this section two SGS models, Smagorinsky and Dynamic Smagorinsky, are employed and simulations are carried out on the selected mesh.

$$\tau_{ij}^s - \frac{1}{3} \tau_{kk}^s \delta_{ij} = \mu_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) = 2\mu_t \bar{S}_{ij}, \quad \mu_t = C_s^2 \rho \Delta^2 |\bar{S}| \quad (10)$$

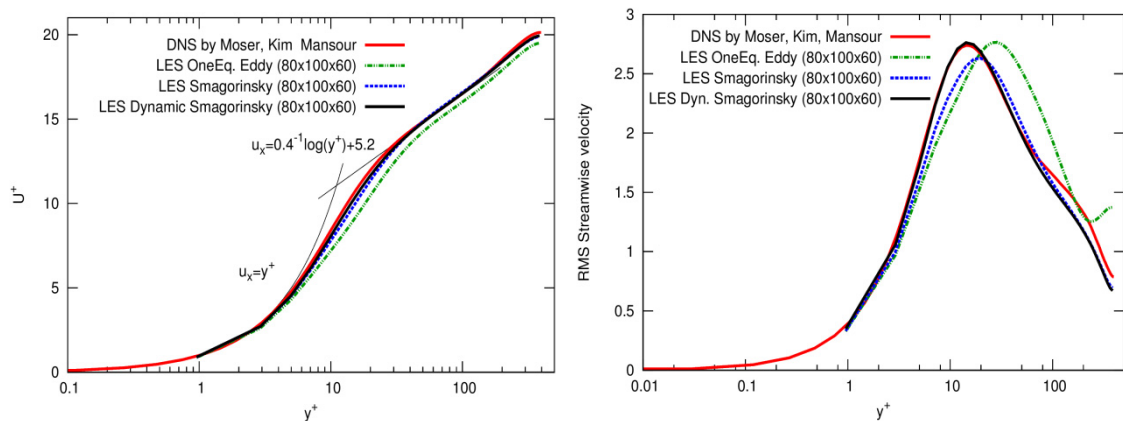


Fig.4. Mean velocity (left) and RMS stream wise velocity (right) profiles in comparison with DNS data [2] for three SGS models

Smagorinsky constant of ≈ 0.11 together with van Driest damping function have been used for Smagorinsky model. Mean velocity profiles in wall units and stream wise RMS velocity values are plotted and compared with DNS results by Moser et al. [2].

As it can be observed in the plotted graphs in Fig. 4, simulations using Dynamic Smagorinsky as SGS model, show great agreement with DNS data. Although the Smagorinsky model seems to represent the main dynamics of the turbulent flow, it is not quite successful. Having no universal value for C_s and not having the capability to account for backscatter effects (where energy is transferred from small unresolved scales to large resolved ones) are some of the drawbacks of the model.

The dynamic procedure that was for the first time introduced by Germano et al. [8] in 1990 produces enhanced results and removes many of difficulties of SGS model. In this approach the model parameter can be calculated at every grid point and at every time step and as one of the results, model parameter is corrected automatically both in bulk flow and also near the wall [9]. Owing to the gained results in comparing three SGS models, Dynamic Smagorinsky is chosen for modeling turbulent pipe flow in the next step.

In a final step, grid resolution study is conducted for Dynamic Smagorinsky model to observe the accuracy for higher resolutions. As it is clear in Fig. 5, the coarse mesh is not efficient and is under resolved. The results calculated on the fine mesh show excellent agreement with mean velocity profile.

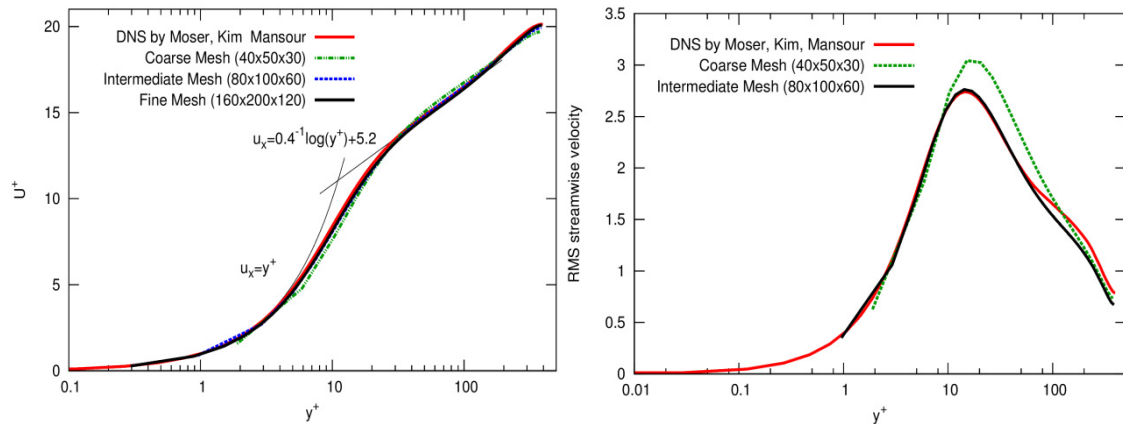


Fig.5. Grid resolution study for Dynamic Smagorinsky model. Mean velocity (left) and RMS stream wise velocity (right) profiles in comparison with DNS data [2]

3. LES of turbulent pipe flow

In the second part of this study LES of incompressible turbulent pipe line fluid flow has been carried out. For this purpose CoLa pipe test facility from author's department has been considered as a benchmark. The existing experimental results of the pipe have been used to improve the solver and validate the accuracy and efficiency of the code.

3.1. Experiment Setup

The test section of the pipe test facility is 27 m long and has an inner diameter of 0.19 m. Air is the working fluid, driven into the pipe by a radial blower with power of 45 KW, providing maximum velocity of 80 m/s and bulk Reynolds number of $3 \times 10^4 \leq Re_b \leq 10^6$. Different components of the test facility are shown in Fig. 6 [3].

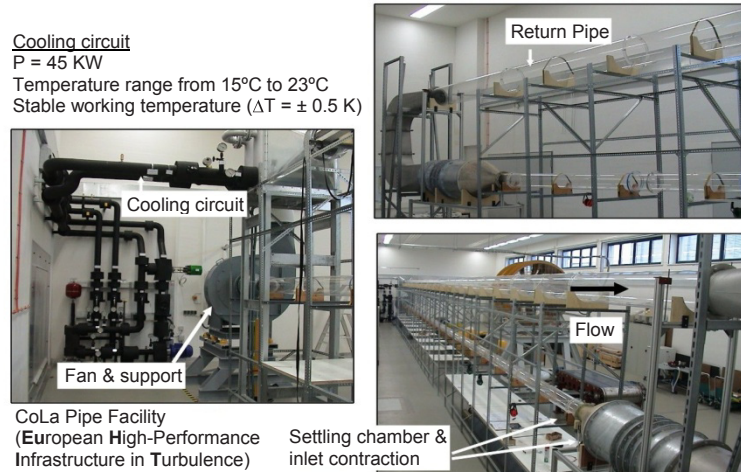


Fig. 6. Pipe test facility at the department of Aerodynamics and Fluid Mechanics of Brandenburg University of Technology Cottbus

3.2. Simulation Setup

LES of the test section of the pipe is performed using OpenFoam at shear Reynolds number of $Re_\tau = 1386$, on mesh resolutions of $(60 \times 100 \times 80)$ and $(120 \times 200 \times 160)$ in (r, θ, z) directions. No slip boundary condition is utilized for the pipe wall. Flow in a pipe segment of 1m length is modeled and periodic boundary conditions are applied in inlet and outlet to simulate fully developed turbulence in the pipe. An initial turbulent velocity field is introduced to the pipe as initial velocity condition to trigger transition. Dynamic Smagorinsky has been implemented as SGS model being the most efficient of the tested models for channel flow in section 2.6. The pipe geometry is presented in Fig.7 and the perturbations in instantaneous velocity field are observable as well as complex structures of the modeled flow near the wall (Fig.7). In the same figure on the left, instantaneous velocity profile along the diameter is plotted together with time averaged velocity profile.

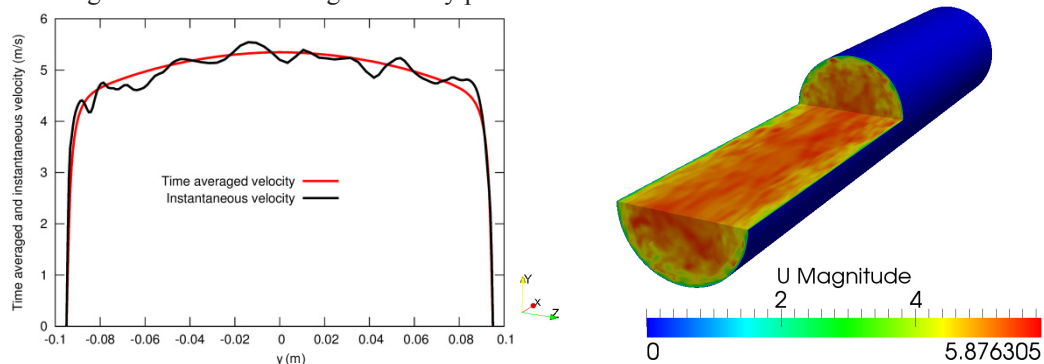


Fig. 7. Pipe geometry (right) and time averaged mean velocity and instantaneous velocity profiles along the pipe diameter (left)

In Fig. 8 experimental and numerical data are compared based on mean velocity profiles for two resolutions in pipe with radius of R [3]. Numerical curves match with the experimental one by trend and quantitative agreement is reached mostly in the viscous and logarithmic layer for the finer mesh. By increasing the resolution, allowing the flow to reach fully developed state and further improvement of the solver, similar agreements between channel flow and DNS data, can be expected between pipe flow simulation and experimental results. The latter, together with calculation and validation of statistical flow quantities, and reaching higher Reynolds numbers are some of the future goals of this study.

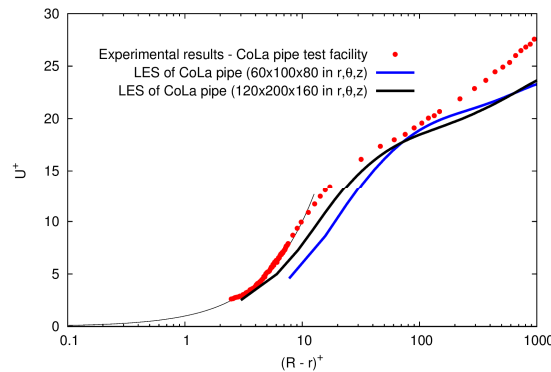


Fig.8. Mean velocity profile of modeled pipe flow for two different grid resolutions and their primary comparison with the corresponding experimental data [3] for $Re_\tau = 1386$, $Re_b = 57352$

Table 2. Air properties used in the modeling [3], CO_2 properties for the same Reynolds number and CO_2 properties in pipe lines in CCS [1]

	Temperature	Density	Kinematic viscosity	Bulk Reynolds	Shear Reynolds	Length/Diameter	Bulk Velocity	Friction Velocity
	T ($^{\circ}C$)	ρ (Kg/m^3)	ν (m^2/s)	Re_b	Re_τ	L/D	u_b (m/s)	u_τ (m/s)
Air	20.61	1.70	1.55×10^{-5}	57352	1386	140	4.68	2.26×10^{-1}
CO_2 (gas)	20	1.83	8.01×10^{-6}	57352	1386	140	2.42	1.16×10^{-1}
CO_2 (liquid)	20	900	8.9×10^{-8}	57352	1386	140	2.6×10^{-2}	1.29×10^{-3}
CO_2 (CCS)	12-44	800-900	0.10×10^{-6}	$(1.5-6) \times 10^7$	-	$L \leq 200$ $D \approx 1.5$	1 - 4	-

The chosen experimental fluid is air being non toxic and due to the simple test facility construction. However the results can be applied to any incompressible fluid by means of the dimensional analysis and physical similarity criteria. The test value of the bulk Reynolds number of $Re_b = 57352$ corresponds to a bulk velocity of 4.68 m/s in air. For the same Re_b , gaseous CO_2 would flow in a pipeline with the same geometrical characteristics at a lower bulk velocity of 2.42 m/s. If liquid CO_2 is transported through the same pipeline at the mentioned Re_b , the reached bulk velocity is much lower being equal to 2.6×10^{-2} m/s. Generally the bulk velocity for liquid CO_2 transportation in the frame work of CCS technology is in the range of 1-4 m/s [1]. To achieve such velocities the order of magnitude for Re_τ has to be increased up to 6×10^7 .

It should be mentioned that by increasing the Reynolds number the computation time increases not only due to flow parameter changes but also due to the need for a finer mesh to resolve the flow. Thus reaching higher Reynolds numbers is regarded as one of the future works to this study.

4. Conclusion

LES of turbulent channel flow and pipe flow was carried out in comparison with existing DNS data from the literature and with experimental measurements. An optimized mesh resolution for channel was chosen. According to the performed grid resolution study, the intermediate mesh with 100 grid points in the wall normal direction and mesh grading towards the walls, provides a reliable accuracy for resolving the flow in regions near the wall as well as the parts in the bulk flow.

Based on the results gained in the channel flow study, One-Equation Eddy Viscosity model can't produce the flow dynamics accurately in the logarithmic layer even in higher resolutions. Smagorinsky SGS model on the other hand proves to be too dissipative especially in the vicinity of the wall. Due to the lack of a universal model constant, the model fails to represent the flow behavior accurately for the viscous and logarithmic layer. The third studied model, Dynamic Smagorinsky, shows excellent agreement with DNS data for the mean velocity profile and stream wise RMS velocity. As a result, this model was employed for modeling turbulent pipe flow. At this stage a relatively good agreement between the primary results and experimental measurements on pipe test facility is observable in the logarithmic and viscous part of mean velocity profile. A higher resolution in radial direction is compulsory to reach more accurate values near the wall. This will be too costly in terms of computation time for higher Reynolds numbers, and therefore use of wall functions can be suggested to improve the results. Reaching higher bulk velocities and Reynolds numbers are included as some of the future perspectives of this study.

Acknowledgements

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